

Localized to extended states transition for two interacting particles in a two-dimensional random potential

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(February 1, 2008)

We show by a numerical procedure that a short-range interaction u induces extended two-particle states in a two-dimensional random potential. Our procedure treats the interaction as a perturbation and solve Dyson's equation exactly in the subspace of doubly occupied sites. We consider long bars of several widths and extract the macroscopic localization and correlation lengths by an scaling analysis of the renormalized decay length of the bars. For $u = 1$, the critical disorder found is $W_c = 9.3 \pm 0.2$, and the critical exponent $\nu = 2.4 \pm 0.5$. For two non-interacting particles we do not find any transition and the localization length is roughly half the one-particle value, as expected.

PACS number(s): 71.30, 72.15 Rn, 71.55 Jv

The interplay of disorder and interactions in electronic systems has been studied intensively within the last two decades [1,2]. Recent experimental results by Kravchenko *et al.* [3] have presented strong evidence for a metal-insulator transition in two-dimensional (2D) high mobility Si metal-oxide-semiconductor field-effect transistors, and have generated a great deal of interest in the problem of the existence of a metallic state in 2D. These results have been confirmed by other workers employing different materials and designs [4]. All these experiments show clear indications that strong electron-electron interactions partially suppress the quantum interference effects responsible for localization. At the same time, the scaling theory of localization including the combined effects of disorder and interactions predicts that a 2D system may remain metallic even in the limit of zero temperature [1].

Direct numerical simulations of the problem are extremely difficult and, at present, we have to conform with solving the simplest related problem, that of just two interacting particles (TIP) in a random potential.

In one-dimensional systems, this TIP problem has attracted a lot of attention since the original works of Dorokhov [5] and Shepelyansky [6]. The problem has been approached from different points of view: by using a Thouless type block-scaling picture [7], by mapping the TIP problem onto a random matrix problem [8], by direct numerical approaches based on the time evolution of wave packets [6,9], by transfer matrix methods [10], by Green function approaches [11,12], by exact diagonalization [13] and by a decimation method [14]. The previous works coincide on the existence of a coherent pair propagation enhancement.

In this Letter we perform a numerical calculation of the TIP problem in a 2D random potential. Our main aim is to establish the existence of extended coherent two-particle pairs. Although in principle this is against the accepted one-particle scaling picture, it should not be very surprising, since 2D is the critical dimension for localization. The consideration, for example, of spin-orbit

coupling effects resulted in a metal-insulator transition [15].

Our algorithm combines an exact implementation of von Oppen *et al.* approach [11] with the scaling procedure of MacKinnon and Kramer [16] for the study of critical properties of disordered systems. We consider long samples and calculate their decay lengths as a function of width and disorder energy. These data support the assumptions made in the scaling theory and prove the existence of a transition from localized to extended states at a finite critical disorder. In addition, to strengthen the validity of our calculations, we performed the same analysis for two non-interacting particles and obtained the expected localization length, i.e., half the value of the one-particle localization length.

Due to the computational effort involved we concentrate in the case of bosons with an on-site interaction, although we expect that our main conclusion is equally valid for fermions. A small test of the dependence of the renormalized decay length with the width of the sample clearly shows the same trend for the existence of a transition as for bosons.

We consider a system of length L and width M described by the standard Anderson-Hubbard hamiltonian for two spinless particles

$$H = t \sum_{\{i,k\},j} |i,j\rangle \langle k,j| + t \sum_{i,\{j,l\}} |i,j\rangle \langle i,l| + \sum_{i,j} |i,j\rangle (\epsilon_i + \epsilon_j) \langle i,j| + U \equiv H_0 + U, \quad (1)$$

where i (and j, k, l) labels the $L \times M$ sites of a square lattice, and ϵ_i is the random site energy chosen from a box distribution with interval $[-W/2, W/2]$. $\{i, k\}$ (and $\{j, l\}$) indicates that the index k (l) runs over the nearest neighbor sites of i (j). The hopping matrix element t is taken equal to -1 and the lattice constant equal to 1, which sets the energy and length scales, respectively. We choose an on-site interaction with matrix elements $\langle i, j | U | k, l \rangle = u \delta_{i,k} \delta_{j,l} \delta_{i,j}$, and use lateral periodic boundary conditions.

To obtain the two-particle decay length ξ of the hamiltonian (1) we focus on the two-particle GF

$$G = (E - H_0 - U)^{-1}. \quad (2)$$

The full GF satisfies Dyson's equation

$$G = G_0 + G_0 U G, \quad (3)$$

where G_0 is the two-particle GF in the absence of interactions. The eigenvectors and eigenvalues of the one-particle problem are enough to construct G_0 [11]. von Oppen *et al.* [11] noted that for a local interaction we can obtain G very efficiently by projecting onto the subspace of doubly occupied sites. This is equivalent to solving first the non-interacting case and considering the interaction as a perturbation, only acting on the subspace of doubly occupied sites. We will refer with a tilde to the matrices restricted to this subspace. Solving Eq. (3) for \tilde{G} , and taking into account that $\tilde{U} = u\mathbb{1}$, we obtain

$$\tilde{G} = (\mathbb{1} - u\tilde{G}_0)^{-1}\tilde{G}_0. \quad (4)$$

This expression can be evaluated exactly by inverting matrices of range equal to the system size, $L \times M$. These matrices are full, all elements are relevant, and their inversion cannot be alleviated by matrix transfer methods.

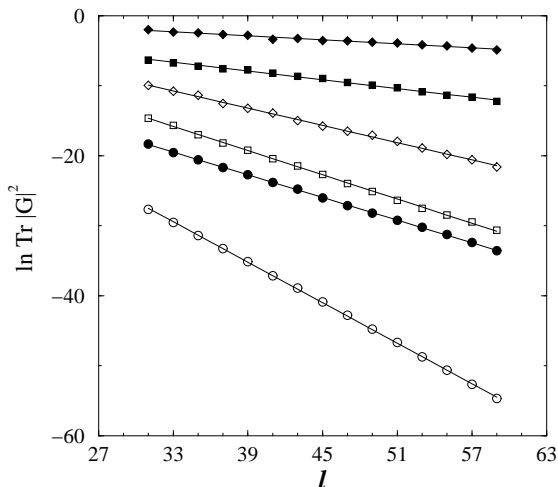


FIG. 1. $\ln \text{Tr} |\tilde{G}|^2$ as a function of l for $W = 6$, and $M=2$ (circles), 4 (squares) and 6 (diamonds). Solid symbols correspond to $u = 1$ and empty symbols to $u = 0$. The straight lines are fits from which we calculate the corresponding decay lengths.

Let us call $\tilde{G}(m_1, n_1; m_2, n_2)$ to the matrix element of the GF between an initial (doubly occupied) site of coordinates (m_1, n_1) , and a final (doubly occupied) site of coordinates (m_2, n_2) . For a given strip of size $L \times M$ we calculate the following trace

$$\ln \text{Tr} |\tilde{G}(l)|^2 \equiv \langle \ln \sum_{i,j} |\tilde{G}(1, i; l, j)|^2 \rangle, \quad (5)$$

with $l \leq L$, and where $\langle \rangle$ denotes an average over the disorder realizations. We ensure that L is large enough to get a linear exponential decay of the trace as a function of l , for any disorder W and width M considered. Once we reach the exponential regime, we fit the data in this regime to a straight line, whose slope α is related to the two-particle decay length ξ_M through $\xi_M = -2/\alpha$.

In Fig. 1 we show $\ln \text{Tr} |\tilde{G}|^2$ as a function of the length l for $M = 2$ (circles), 4 (squares) and 6 (diamonds). Solid symbols correspond to the interacting case and empty symbols to $u = 0$. Each data is obtained by averaging over at least 300 configurations. The disorder strength is $W = 6$, which for the interacting case already lies in the extended regime, as we will see. We can note that a linear exponential decay is well established in all cases considered. Strictly speaking our results constitute a lower bound for the decay length, but the quality of the exponential decay implies that a larger decay length would have a very small weight and so would correspond to very rare two-particle states. To further check the validity of our results, we will apply the same procedure to non-interacting particles and we will see that we obtain the expected results as compared with transfer matrix calculations with very long bars [16,17], which are not feasible for the interacting problem.

Finite-size scaling analysis [16,17] states that the renormalized decay length ξ_M/M is a function of a single parameter ξ/M ,

$$\xi_M/M = f(M/\xi). \quad (6)$$

The scaling parameter ξ is the two-particle localization length in the localized regime, and the two-particle correlation length in the extended regime. Equation (6) implies that in a log-log plot of ξ_M/M versus M all data should collapse in a common curve when translated by an amount $\ln \xi(W)$ along the horizontal axis. This curve has a single branch when there is no transition, while it develops two separate branches when a transition is present. The main aim of this paper is to discern whether ξ_M/M collapses into a single or into a double branched curve.

In Fig. 2, we show the raw data for ξ_M/M as a function of the system width M on a double logarithmic scale for different values of the disorder. The on-site energy is $u = 1$ and the disorder energies range between $W = 6$ and 15, as indicated in the figure. All data were obtained by averaging over a number of disorder realizations ranging between 300, for the largest M , and 1000, for $M = 2$. We consider the center of the band ($E = 0$), and a length $L = 62$. The fact that ξ_M/M increases with M for small values of W , while it decreases for large values of W is a clear sign of the presence of a transition.

A scaling analysis of the data shown in Fig. 2 is depicted in Fig. 3, where we have overlapped all points on one curve within the accuracy of the data, by shifting the data horizontally by a disorder dependent amount, which

is determined by a least-square fit procedure [16]. Fitting the data set for $W = 15$ and M between 4 and 10 to the form $\xi_M = \xi + A/M$ we obtain the localization length for this disorder $\xi(15) = 2.1 \pm 0.1$, which enables us to establish the absolute scale of $\xi(W)$. As there is practically no overlap between the two branches, we have to obtain the absolute scale for the upper branch by assuming that the scaling parameter diverges symmetrically from above and below at the transition. The existence of two branches is a clear indication of a transition. We will see later on how for the non-interacting case we obtain only one branch, as expected.

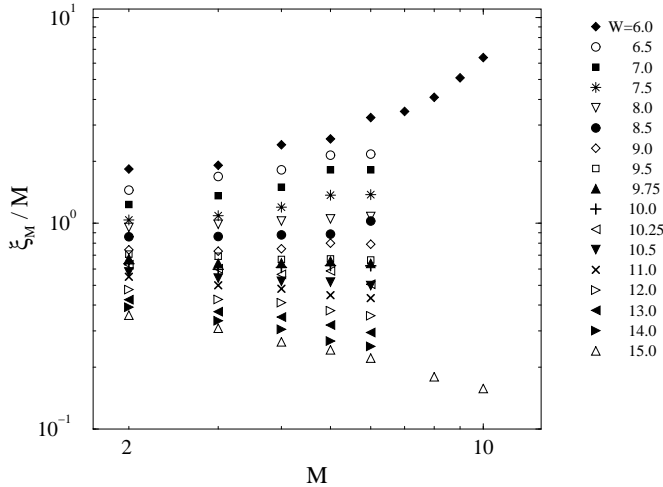


FIG. 2. ξ_M/M versus M on a double logarithmic scale for two-interacting particles with $u = 1$ and for the indicated values of the disorder parameter W .

In order to obtain the critical disorder W_c and the critical exponent ν , we performed an statistical analysis of the data in the range $8 \leq W \leq 10.5$ with the Levenberg-Marquardt method for nonlinear least-squares models. The most likely fit is determined by minimizing the χ^2 statistic of the fitting function, which we choose to be of the form

$$\frac{\xi_M}{M} = \sum_{i=0}^3 A_i (W - W_c)^i M^{i/\nu}. \quad (7)$$

The critical disorder found for $u = 1$ is $W_c = 9.3 \pm 0.2$, and the corresponding critical exponent is equal to $\nu = 2.4 \pm 0.5$. The error bar results mainly from the uncertainty in the critical disorder.

The amount by which we must shift the raw data of Fig. 2 to get the universal curve of Fig. 3 gives us the scaling parameter ξ as a function of disorder for TIP. In the inset of Fig. 3 we plot the disorder dependence of $\log \xi$ for $u = 1$ and the center of the band ($E = 0$).

It should be emphasized that we only demonstrate the existence of correlated two-particle extended states. Probably, there exist many more uncorrelated localized

states where the two particles are away from each other. Our procedure picks up the longest decay length, at the energy considered, which is associated with the most delocalized states.

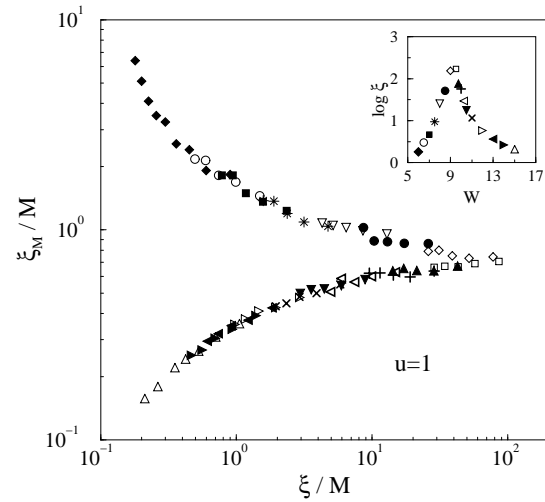


FIG. 3. Log-log plot of ξ_M/M as a function of ξ/M for the data represented in Fig. 2. Inset: disorder dependence of the scaling parameter ξ .

The results for $u = 0$ are qualitatively different from those for $u = 1$. In the non-interacting case, ξ_M/M decreases with increasing M for all values of the disorder W considered, and so there appears only one branch in the scaling procedure. In Fig. 4 we represent ξ_M/M as a function of the scaling parameter ξ divided by M . The upper inset shows the disorder dependence of $\log \xi$. For comparison we also represent the one-particle localization length divided by two $\xi_1/2$ (solid line), which is the expected result for relatively strongly localized systems at $u = 0$. We take for ξ_1 the value reported by MacKinnon and Kramer [16]. The agreement between our results and $\xi_1/2$ is a positive check of the validity of our method of calculation. In the range of validity of our results we do not obtain any artificial transition for non-interacting particles, as previously reported for one particle in 2D [18], due to a different interpretation of the raw data. We use MacKinnon and Kramer's [16] interpretation, which produces no artificial transition either for the one-particle problem or for our two-particle states calculations. As a further check, we have applied our method to the well studied 1D problem. In the lower inset of Fig. 4 we show ξ versus disorder on a double logarithmic scale for two interacting (solid circles) and two non-interacting (empty circles) bosons in 1D. The straight line corresponds to $\xi_1/2$, where the one-particle localization length ξ_1 is taken equal to $105/W^2$. We consider samples with 500 sites. Our results agree with well established previous calculations [8,12,14].

The extension of our results to the case of degenerate

electrons, so that can be applied to explain the transitions found experimentally in Refs. [3] and [4] and to the scaling theory of localization including interactions [1], is a very difficult problem. In three-dimensional systems, Imry [7] argued about the existence of an effective two-particle mobility edge that would approach the Fermi energy faster than the single-particle mobility edge. Our results in 2D could be interpreted as due to the existence of a two-particle mobility edge which overcomes the single-particle mobility edge at $W = 0$. Before arguing in favor of a transition in 2D degenerate disordered systems, one should estimate the lifetime of the coherent pairs. It is not clear how fast our two-particle states would decay to lower energy excitations. In the case of degenerate electrons with long-range Coulomb interactions, Talamantes *et al.* [19] reported an increase of the localization length with respect to the non-interacting case, but they only considered the strongly localized regime.

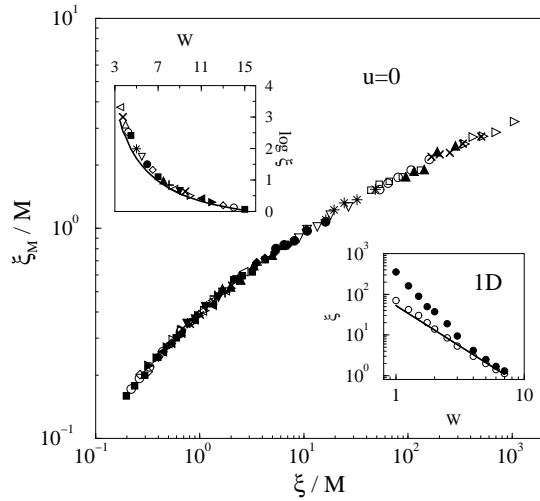


FIG. 4. Log-log plot of ξ_M/M as a function of ξ/M for the non-interacting case. Upper inset: disorder dependence of $\log \xi$ along with the one-particle localization length divided by two, $\xi_1/2$ (solid line). Lower inset: ξ versus W for two interacting (solid circles) and two non-interacting (empty circles) bosons in 1D. The straight line corresponds to $\xi_1/2 = 105/2W^2$.

To summarize, we have calculated numerically the decay length of TIP in 2D disordered bars of several widths. The results are consistent with the assumption of a scaling hypothesis. Through a scaling analysis of the data for $u = 1$, we proved that there is a localized to extended transition at a critical disorder $W_c \approx 9.3$. The critical exponent for the localization length is $\nu \approx 2.4$. Our method clearly indicates the existence of delocalized states for small disorders, although the values of the critical disorder and exponent can appreciably change when larger system sizes can be handled.

We would like to acknowledge financial support from

the Spanish DGES, project number PB96-1118.

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